Verification and first ICF-related simulations with iFP

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Outline

- Discrete mass, momentum, and energy conservation strategy
  - Collision operator
  - Vlasov equation with grid adaptivity

- Verification studies
  - Single species standing shock
  - Two species shock break out through density jump/drop
  - Shock reflection in planar geometry
  - Two species high Z interface mixing
  - Spherical geometry converging shock problem
- Next steps

Rosenbluth-Fokker-Planck collision operator: simultaneous conservation of mass, momentum, and energy

Rosenbluth-FP collision operator: conservation properties results from symmetries

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

Mass

$$\langle 1, C_{\alpha\beta} \rangle_{\vec{v}} = 0 \qquad \Rightarrow \qquad \boxed{\left. \vec{J}_{\alpha\beta,G} - \vec{J}_{\alpha\beta,H} \right|_{\partial\vec{v}} = 0}$$

Momentum

$$m_\alpha \langle \vec{v}, C_{\alpha\beta} \rangle_{\vec{v}} = -m_\beta \langle \vec{v}, C_{\beta\alpha} \rangle_{\vec{v}} \Rightarrow \boxed{\left\langle 1, J^{\|}_{\alpha\beta,G} - J^{\|}_{\beta\alpha,H} \right\rangle_{\vec{v}} = 0}$$

Energy

$$m_\alpha \left\{ \left\langle v^2, C_{\alpha\beta} \right\rangle_{\vec{v}} \right\} = -m_\beta \left\{ \left\langle v^2, C_{\beta\alpha} \right\rangle_{\vec{v}} \right\} \Rightarrow \boxed{\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0}$$

2V Rosenbluth-FP collision operator: numerical conservation of energy

- The symmetry to enforce is:

$$\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0$$

- Due to discretization error:

$$\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = \boxed{\mathcal{O}\left(\Delta_v\right)}$$

- Introduce a constraint coefficient:

$$\left\langle \vec{v}, \boxed{\gamma_{\beta\alpha}} \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0 \qquad \gamma_{\beta\alpha} = \frac{\left\langle \vec{v}, \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}}}{\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} \right\rangle_{\vec{v}}} = 1 + \boxed{\mathcal{O}\left(\Delta_v\right)}$$

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\boxed{\gamma_{\alpha\beta}} \vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

[1] W.T. Taitano, JCP 297, pp.357-380 (2015)

2V Rosenbluth-FP collision operator: numerical conservation of momentum+energy

- Simultaneous conservation of momentum and energy:

$$\boxed{C_{\alpha\beta} = \Gamma_{\alpha\beta}\nabla_v \cdot \left[\boxed{\underline{\underline{\eta}}_{\alpha\beta}} \cdot \vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta}\vec{J}_{\alpha\beta,H}\right]}$$

with:

$$\underline{\underline{\eta}}_{\alpha\beta} = \begin{bmatrix} \gamma_{\alpha\beta} + \epsilon_{||,\alpha\beta} & 0 \\ 0 & \gamma_{\alpha\beta} \end{bmatrix}$$

Momentum

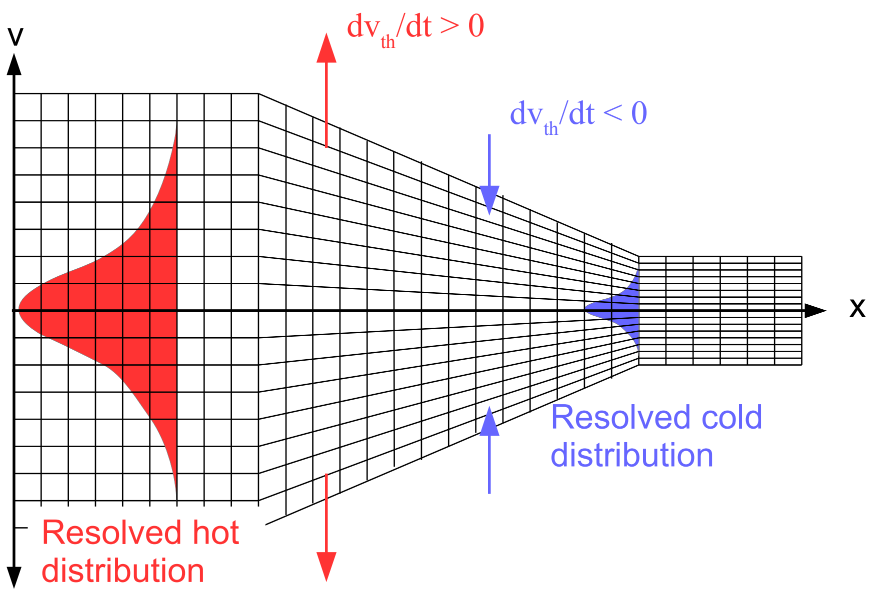
Energy

$$\gamma_{\alpha\beta} = \frac{\left\langle \vec{v}, \vec{J}_{H,\beta\alpha} \right\rangle_{\vec{v}} - \boxed{\epsilon^{+}_{\alpha\beta,||}} \left\langle \vec{v}, \vec{J}_{G,\alpha\beta} \right\rangle^{+\infty}_{\vec{v}-\vec{u}}}{\left\langle \vec{v}, \vec{J}_{G,\alpha\beta} \right\rangle_{\vec{v}}}$$

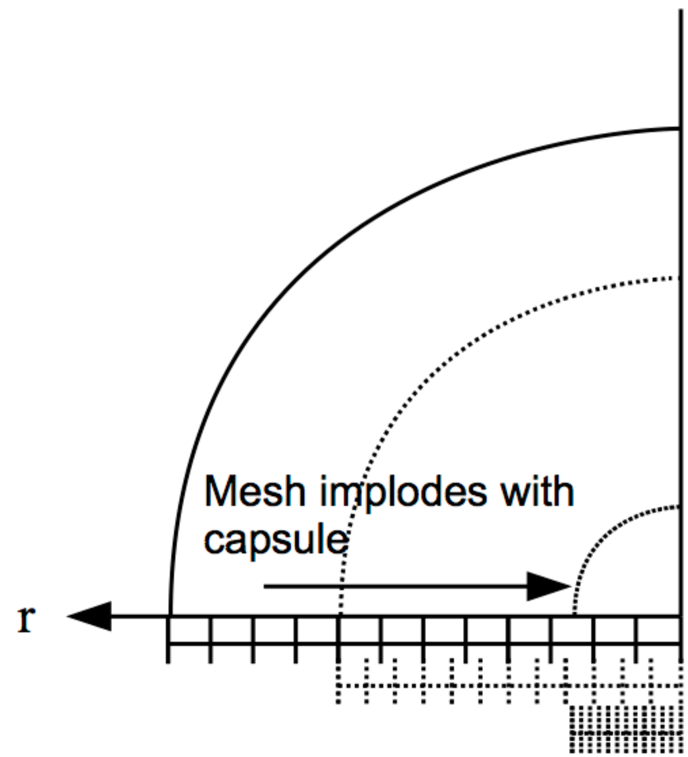
$$\epsilon_{\alpha\beta} = \left\{ \begin{array}{ll} \epsilon^{-}_{||,\alpha\beta} = 0 & \text{if } v_{||} - u_{avg,||,\alpha\beta} \leq 0 \\ \epsilon^{+}_{||,\alpha\beta} = \dfrac{\left\langle 1, J_{H,\beta\alpha,||} \right\rangle_{\vec{v}} - \boxed{\gamma_{\alpha\beta}} \left\langle 1, J_{G,\alpha\beta,||} \right\rangle_{\vec{v}}}{\left\langle 1, J_{G,\alpha\beta,||} \right\rangle^{+\infty}_{\vec{v}-\vec{u}_{avg,\alpha\beta}}} & \text{else} \end{array} \right\}$$

Vlasov equation: Inertial term simultaneous conservation of mass, momentum, and energy

Adaptive grids: v_{th} adaptivity in velocity and Lagrangian mesh in position



v_{th} adaptive Mesh



Adaptivity introduces inertial terms in the conservation equation

- VRFP equation in transformed coordinates

$$\partial_t \left(\sqrt{g_v} J_{r\xi} f_\alpha\right) + \partial_\xi \left(\sqrt{g_v} v_{th,\alpha} \left[\widehat{v}_{||} - \boxed{\widehat{\dot{r}}_\alpha}\right] f_\alpha\right) +$$

$$\partial_{\widehat{v}_{||}} \left(J_{r\xi} \sqrt{g_v} \boxed{\widehat{\dot{v}}_{||}} f_\alpha\right) + \partial_{\widehat{v}_\perp} \left(J_{r\xi} \sqrt{g_v} \boxed{\widehat{\dot{v}}_\perp} f_\alpha\right) = J_{r\xi} \sqrt{g_v} \sum_\beta^{N_s} C_{\alpha\beta}\left(f_\alpha, f_\beta\right)$$

$$\boxed{\widehat{\dot{v}}_{||}} = -\boxed{\frac{\widehat{v}_{||}}{2} \left(v_{th,\alpha}^{-2} \partial_t v_{th,\alpha}^2 + J_{r\xi}^{-1} \left(\widehat{v}_{||} - \widehat{\dot{x}}\right) v_{th,\alpha}^{-1} \partial_\xi v_{th,\alpha}^2\right)} + \frac{\widehat{v}_\perp^2 v_{th,\alpha}}{r} + \frac{q_\alpha E_{||}}{J_{r\xi} m_\alpha v_{th,\alpha}}$$

$$\boxed{\widehat{\dot{v}}_\perp} = -\boxed{\frac{\widehat{v}_\perp}{2} \left(v_{th,\alpha}^{-2} \partial_t v_{th,\alpha}^2 + J_{r\xi}^{-1} \left(\widehat{v}_{||} - \widehat{\dot{x}}\right) v_{th,\alpha}^{-1} \partial_\xi v_{th,\alpha}^2\right)} - \frac{\widehat{v}_{||} \widehat{v}_\perp v_{th,\alpha}}{r}$$

Inertial terms due to v_{th} adaptivity and Lagrangian mesh

FP equation with adaptivity in velocity space: Temporal inertial terms

- Focus on temporal inertial terms due to normalization wrt $v_{th}(r,t)$ (OD):

$$\boxed{v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) = 0}$$

- Mass conservation can be trivially shown by 0^{th} velocity space moment:

$$v_{th}^2 \frac{\partial n_\alpha}{\partial t} = 0$$

Find symmetry in continuum and enforce via using discrete nonlinear constraints (similar to collisions)

$$v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) = 0$$

Rewrite as:

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\boxed{\widehat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right)} \right] = 0$$

Energy conservation shown from 2nd velocity moment:

$$\frac{\partial U_\alpha}{\partial t} = 0$$

This property relies on: $\boxed{\left\langle \widehat{v}^2, \widehat{f}_\alpha + \frac{1}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0}$

This property must be enforced numerically:

$$\left\langle \widehat{v}^2, \widehat{f}_\alpha + \frac{\gamma_{t,\alpha}}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0 \qquad \gamma_{t,\alpha} = - \frac{\left\langle \frac{\widehat{v}^2}{2}, \widehat{f}_\alpha \right\rangle_{\widehat{v}}}{\left\langle \frac{\widehat{v}^2}{2}, \frac{1}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\widehat{v}}}$$

All conservation law can be enforced via recursive application of chain rule

$$v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha\right) = 0$$

- Rewrite as:

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha\right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \gamma_{t,\alpha} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha\right)\right] + \xi_{t,\alpha} = 0$$

Truncation error

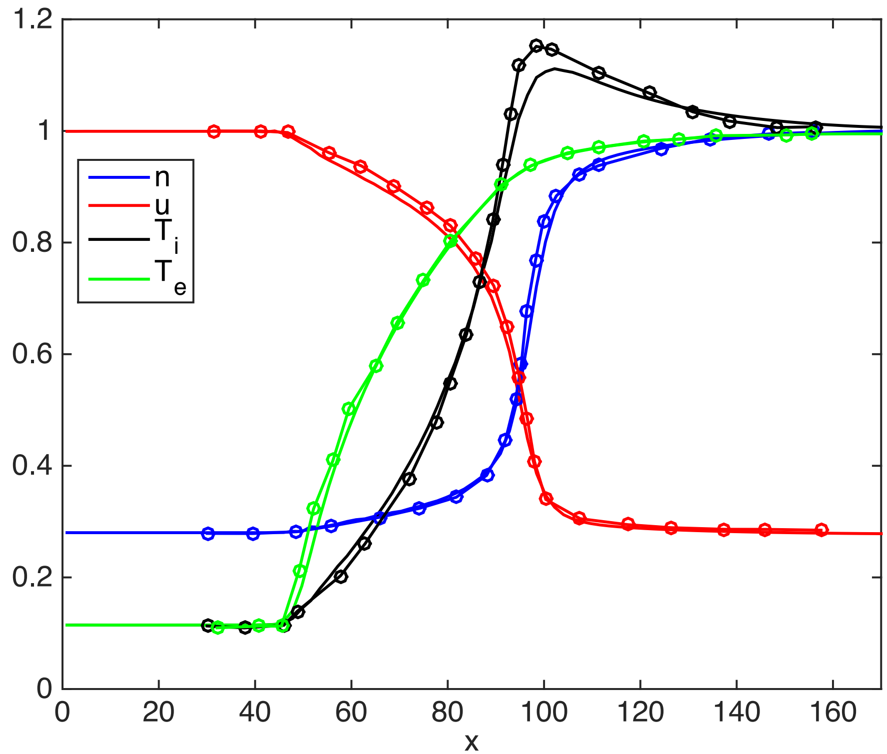
$$\begin{aligned}\xi_{t,\alpha} = {} & v_{th,\alpha} \left\{\partial_t \left(v_{th,\alpha} \widehat{f}_\alpha\right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\underline{\underline{\Upsilon}}_{t,\alpha} \widehat{\vec{v}} \widehat{f}_\alpha\right)\right]\right\} + \eta_{t,\alpha} \\ & - \left\{\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha\right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha\right)\right]\right\},\end{aligned}$$

$$\begin{aligned}\eta_{t,\alpha}(v) = {} & \left\{v_{th,\alpha}^2 \partial_t \widehat{f}_\alpha - \partial_t v_{th,\alpha}^2 \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha\right)\right\} \\ & - v_{th,\alpha} \left\{\partial_t \left(v_{th,\alpha} \widehat{f}_\alpha\right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha\right)\right]\right\}\end{aligned}$$

[2] W.T. Taitano, JCP accepted (2016)

Verification studies

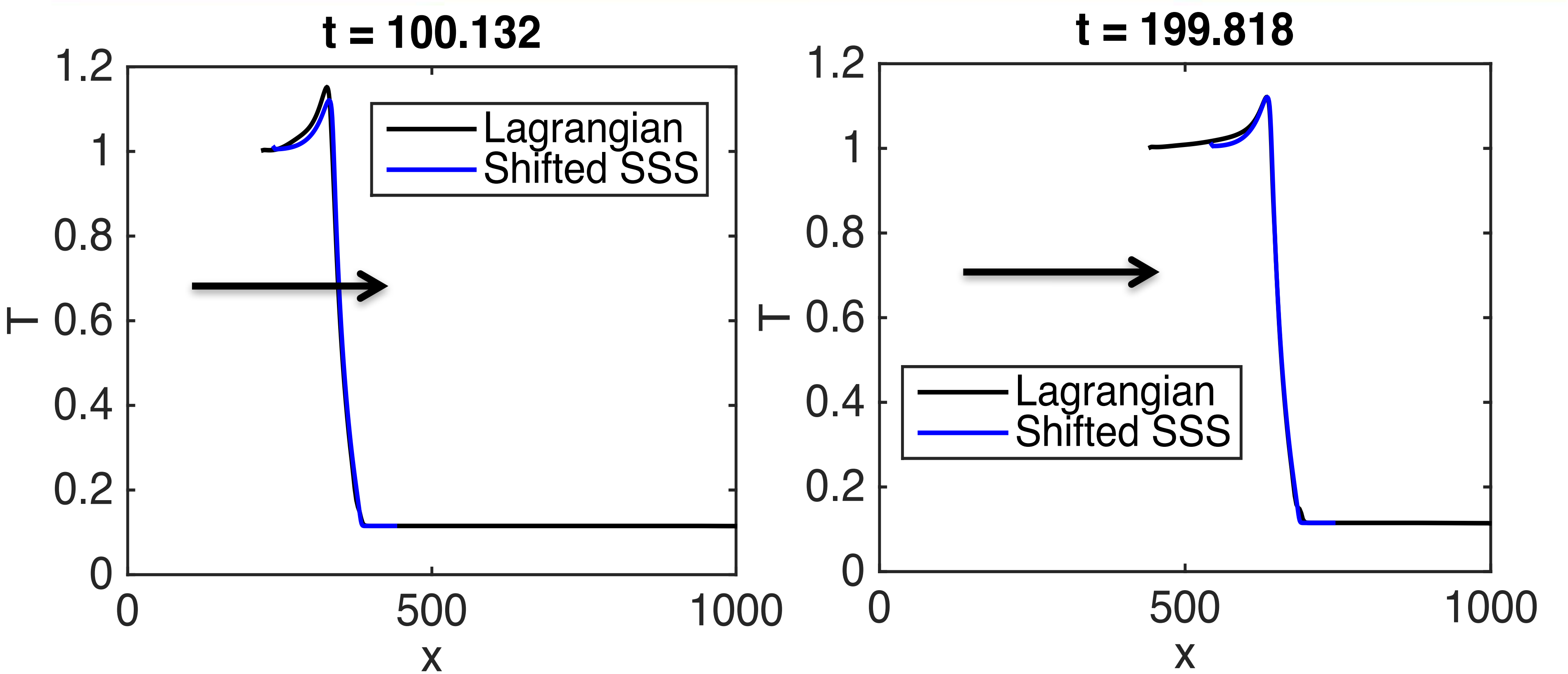
Planar M=5 standing shock [3]



M=5 planar steady state shock solution (SSS) comparison between iFP (solid line) and reference solution from [3] (open circles).

[3] F. Vidal et al., PoF B, 3182 (1993)

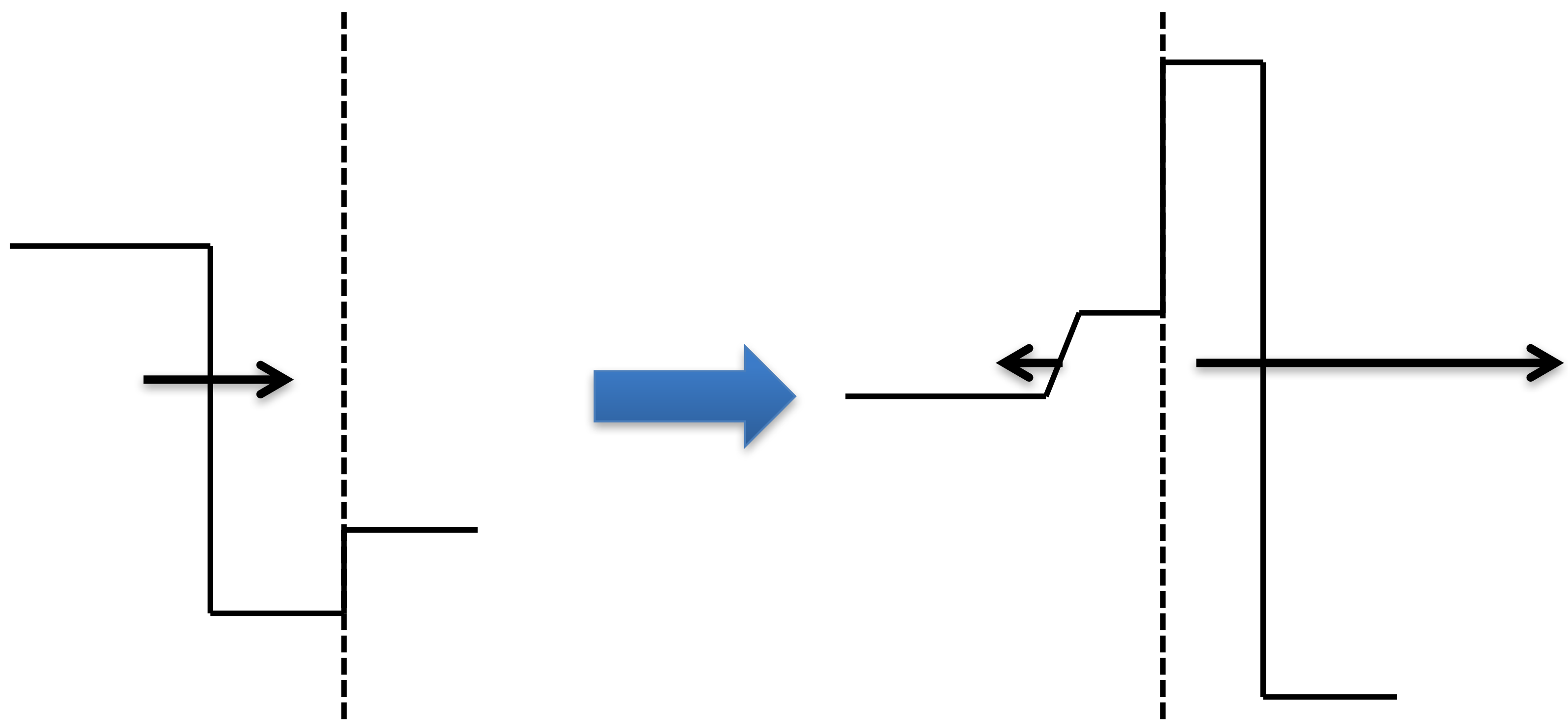
Shock-tracking Lagrangian mesh



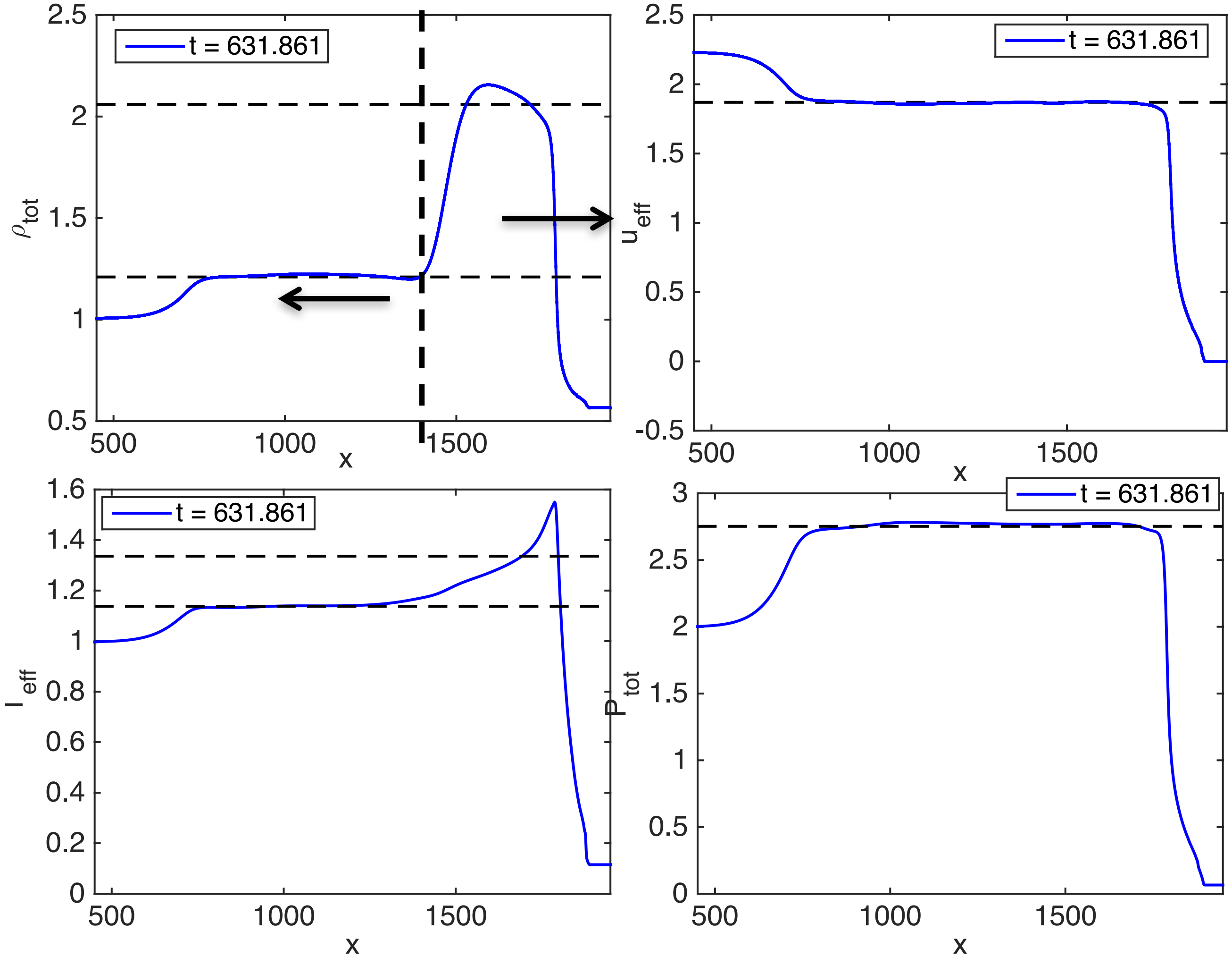
Test of Lagrangian mesh capability for a M=5 shock in lab frame. A good agreement in solutions between Lagrangian mesh and SSS is achieved.

Planar D-H shock across density jump

- Key features
  - Reflective and transmitted shock
  - Reflective is weaker and transmitted is stronger than initial shock

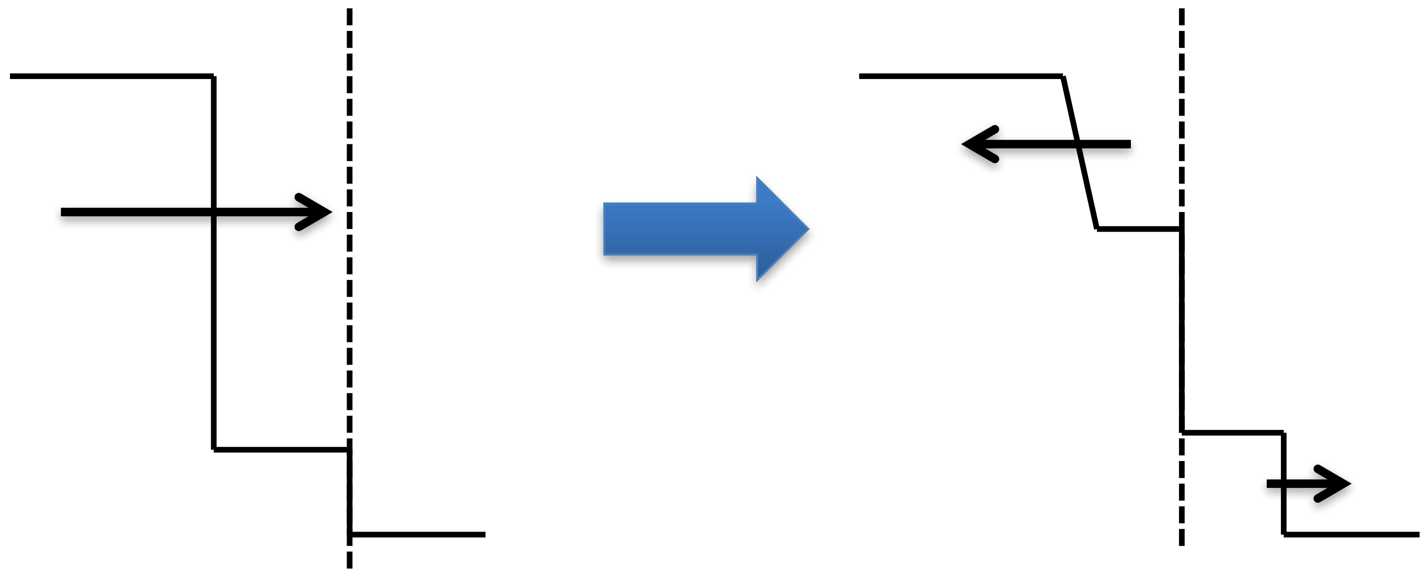


iFP captures jump conditions correctly

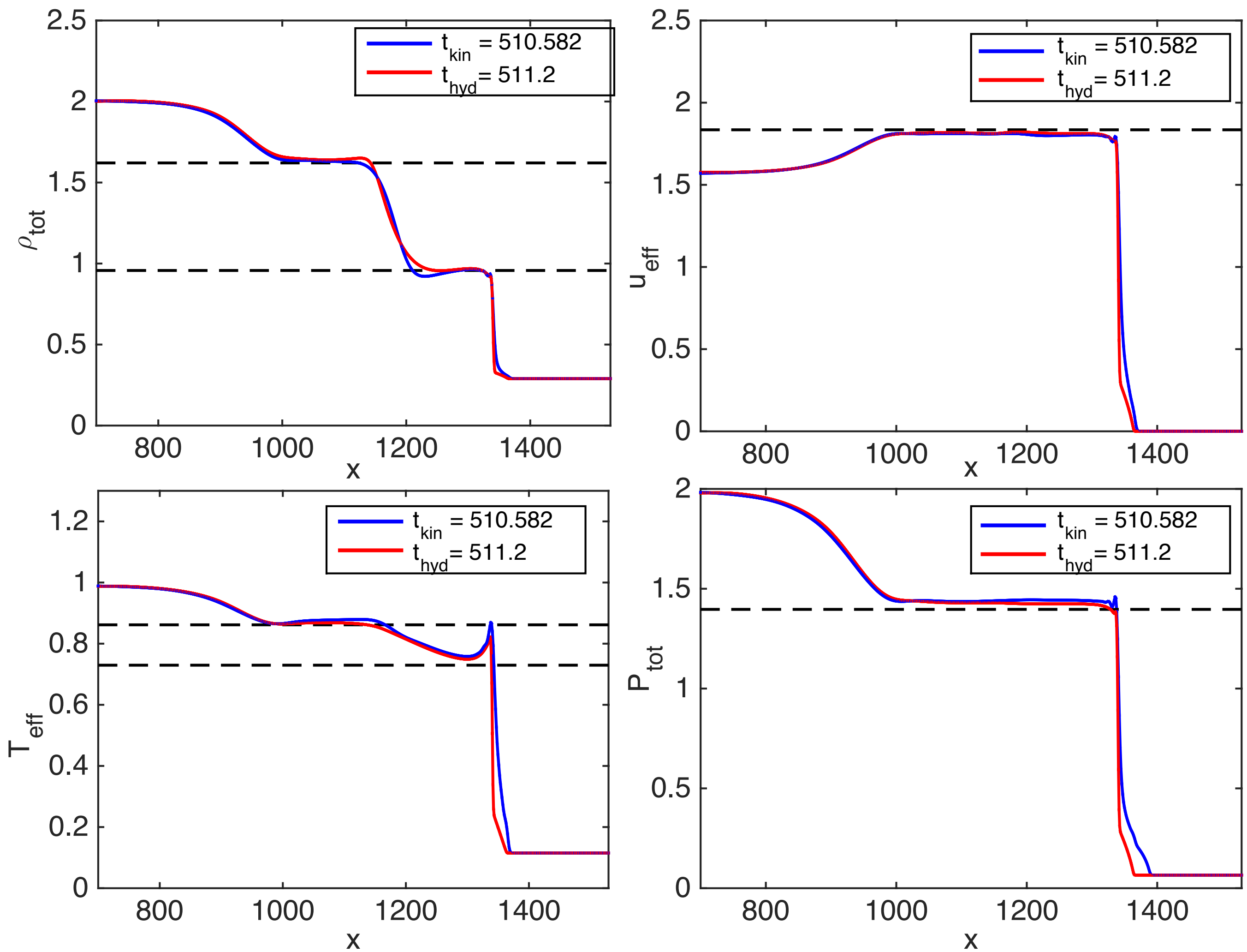


Planar D-H shock across density drop

- Key features
  - Rarefaction wave and transmitted shock
  - Transmitted shock is weaker than initial shock

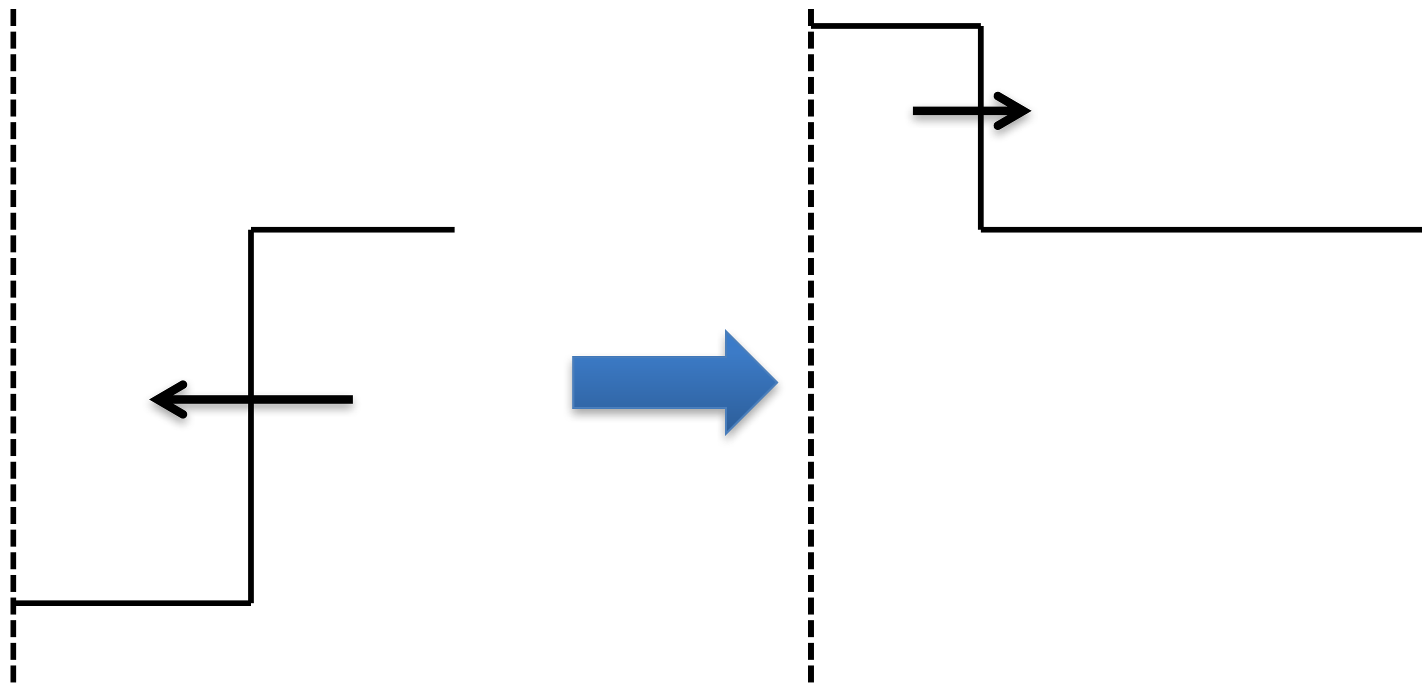


iFP captures jump conditions correctly

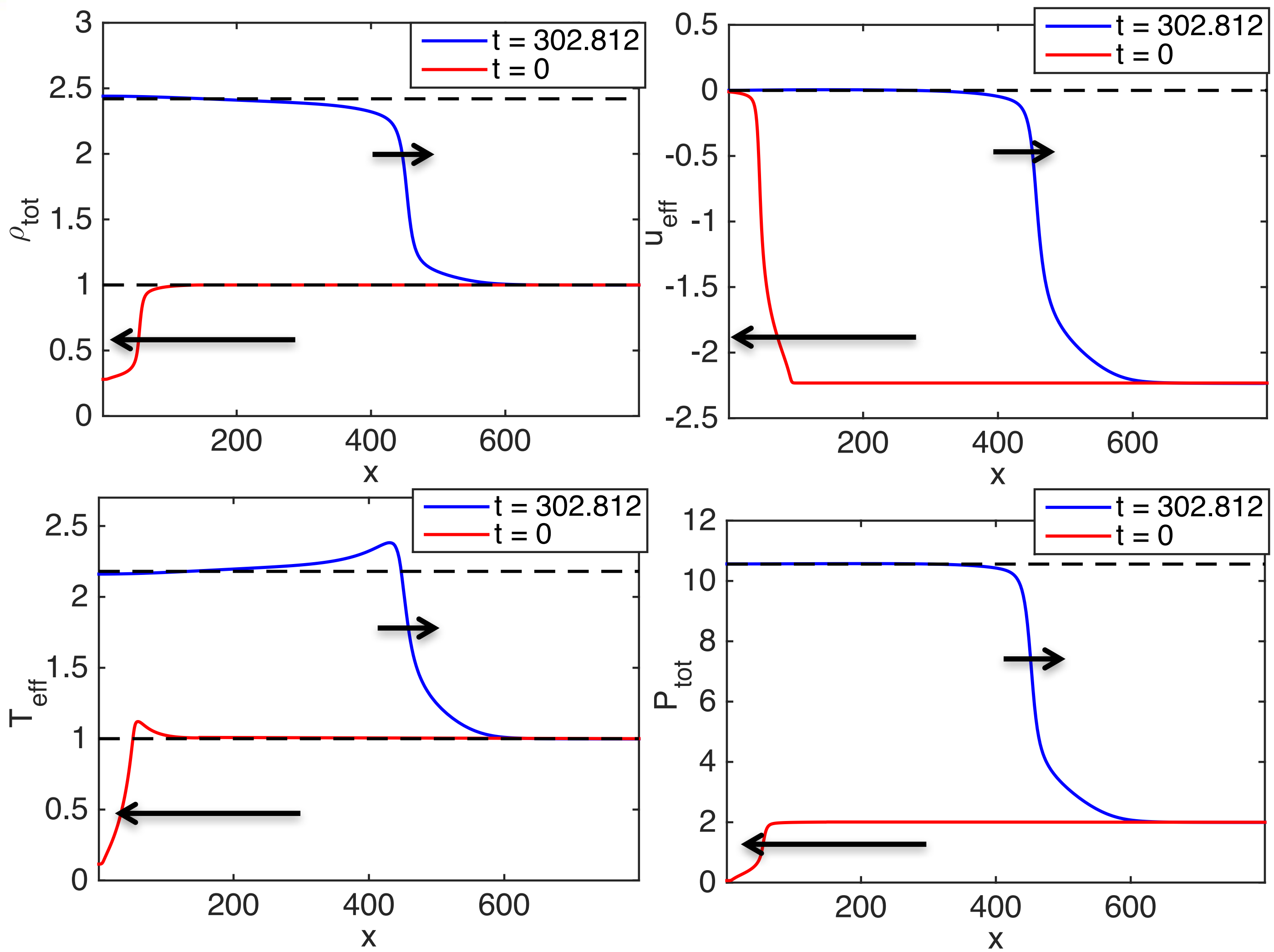


Planar reflective shock calculation

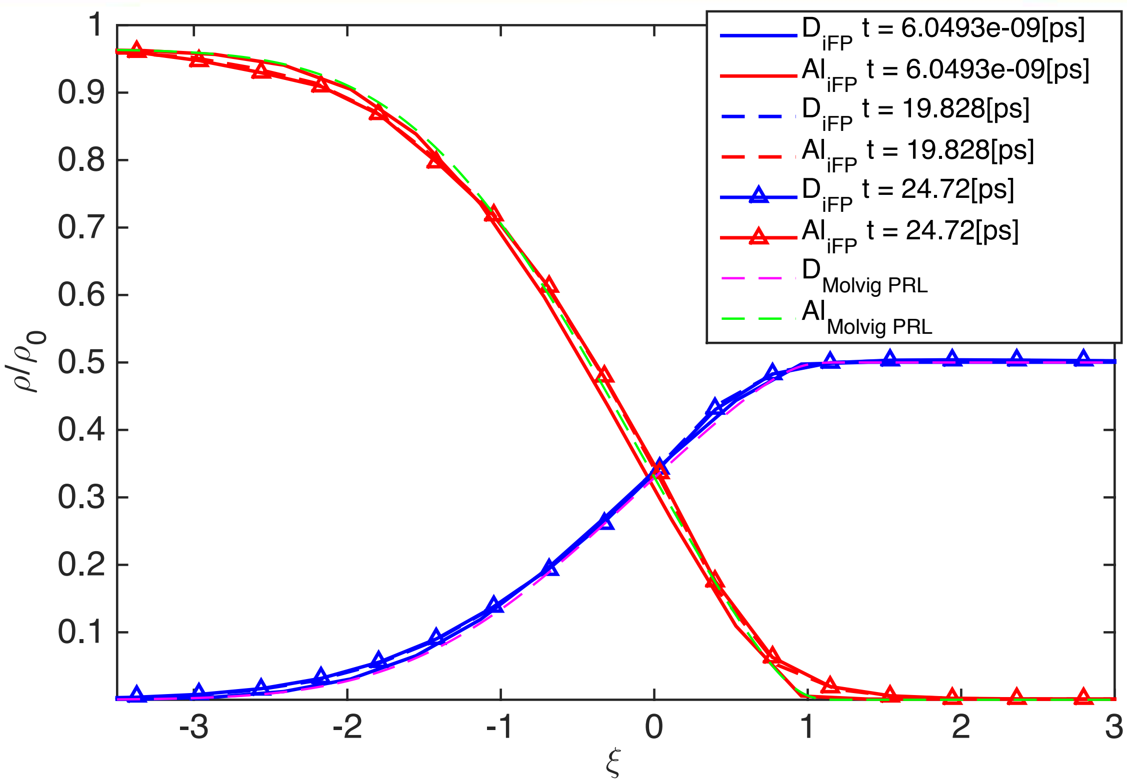
- Key features: Reflective shock weaker than initial shock



iFP predicts the jump condition for reflective shock correctly



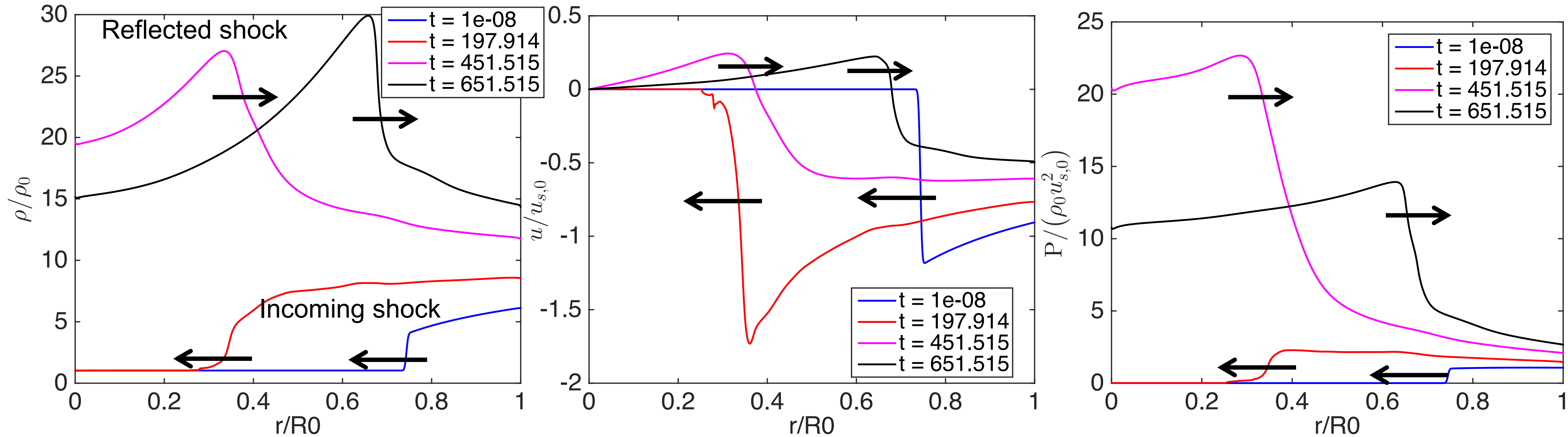
1D2V: D-Al interface mixing [4]

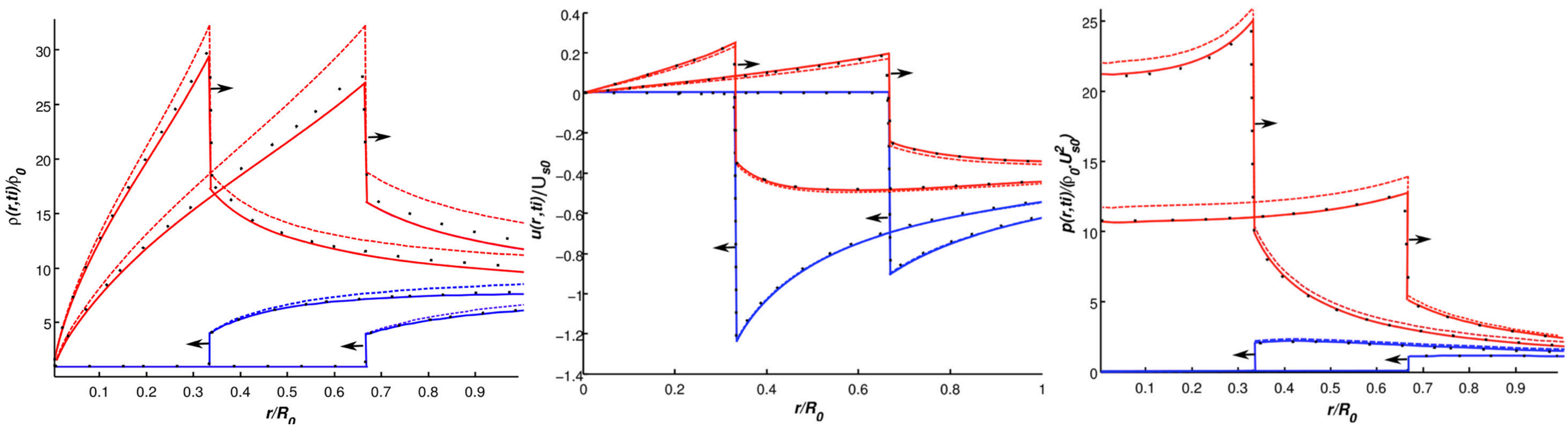


Correct self similar solution [4] obtained for t>>τ_{col}.
Test of implicit solver with D-Al interface problem with $\Delta t = 4\text{x}10^4\ \tau_{col}$.

[4] K. Molvig et al., PRL 113, 145001 (2014)

Spherical geometry:
Guderley problem with finite Mach # [5]





[5] A. Vallet et al., PoP 20, 082702 (2013)

Future (physics) work

- Fuel stratification in planar shock (currently ongoing)
- Spherical implosion with fuel B.C. from hydro calculation (possible now)
- With improved preconditioning, a self-consistent evolution of fuel-pusher in capsule possible (summer~fall 2016)

Questions?